Magnetic-dipole transition probabilities in B-like and Be-like ions

I. I. Tupitsyn,[1] A. V. Volotka,[1,2] D. A. Glazov,[1] V. M. Shabaev,[1,3] G. Plunien,[2] J. R. Crespo López-Urrutia,[4] A. Lapierre,[4] and J. Ullrich[4]

[1]*Department of Physics, St. Petersburg State University, Oulianovskaya 1, Petrodvorets, 198504 St. Petersburg, Russia*

[2]*Institut für Theoretische Physik, TU Dresden, Mommsenstraße 13, D-01062 Dresden, Germany*

[3]*Max-Planck Institut für Physik Komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany*

[4]*Max-Planck Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg, Germany*

(Received 11 September 2005; published 14 December 2005)

The magnetic-dipole transition probabilities between the fine-structure levels $(1s^22s^22p)\ ^2P_{1/2}-^2P_{3/2}$ for B-like ions and $(1s^22s2p)\ ^3P_1-^3P_2$ for Be-like ions are calculated. The configuration-interaction method in the Dirac-Fock-Sturm basis is employed for the evaluation of the interelectronic-interaction correction with negative-continuum spectrum being taken into account. The $1/Z$ interelectronic-interaction contribution is derived within a rigorous QED approach employing the two-time Green function method. The one-electron QED correction is evaluated within framework of the anomalous magnetic-moment approximation. A comparison with the theoretical results of other authors and with available experimental data is presented.

DOI: 10.1103/PhysRevA.72.062503 PACS number(s): 32.70.Cs

I. INTRODUCTION

During the last years, the precision of measurements of magnetic-dipole ($M1$) transitions between the fine-structure levels in highly charged ions has been continuously increased [1–8]. Since in some cases the $M1$ transitions are sufficiently sensitive to relativistic-correlation and quantum-electrodynamic (QED) effects, this provides good prospects for probing their influences on atomic transition probabilities.

To date, a vast number of theoretical calculations of $M1$-transition probabilities between the fine-structure levels in highly charged ions have been performed (see, e.g., Refs. [9–11]). However, none of these works have provided a systematic analysis of various effects on the transition probability. Such an analysis for the $(1s^22s^22p)\ ^2P_{1/2}-^2P_{3/2}$ transition in B-like ions and for the $(1s^22s2p)\ ^3P_1-^3P_2$ transition in Be-like ions is given in the present paper.

To calculate the decay rate one requires knowledge of the transition energy and the matrix element of the transition operator. Within this work we employ experimental values of the transition energy, which are measured accurately enough for the ions under consideration.

To analyze the influence of various effects, we decompose the transition probability $W^{i\to f}$ into several terms,

$$W^{i\to f} = W^{i\to f}_{\rm nr} + \Delta W^{i\to f}_{\rm D} + \Delta W^{i\to f}_{\rm CI} + \Delta W^{i\to f}_{\rm neg} + \Delta W^{i\to f}_{\rm QED} + \Delta W^{i\to f}_{\rm freq}.$$

Here $W^{i\to f}_{\rm nr}$ represents the nonrelativistic $M1$-transition probability derived employing the LS-coupling scheme. Within the LS-coupling scheme, the amplitude of the magnetic-dipole transition is nonzero only between the fine-structure levels and depends on the quantum numbers L, S, and J of the initial and the final state [12]. This implies that the contribution of the interelectronic interaction vanishes in the nonrelativistic limit. The explicit expression for $W^{i\to f}_{\rm nr}$ is presented in Sec. II.

The relativistic correction $\Delta W^{i\to f}_{\rm D}$ is obtained by employing the one-electron Dirac wave functions for the initial and final states. For the relativistic case the interelectronic-interaction contribution is nonzero, but it is generally suppressed by a factor $(\alpha Z)^2/Z$. For instance, in case of B-like Ar it amounts to about 0.1%. The interelectronic-interaction correction is, however, rather important for the $(1s^22s2p)\ ^3P_1-^3P_2$ transition in Be-like ions, where the terms $^3P_1$ and $^1P_1$ are strongly mixed. In this investigation two approaches are employed for evaluating the interelectronic-interaction correction. The first one is based on the configuration-interaction (CI) method in the Dirac-Fock-Sturm basis, whereas the second one employs perturbation theory with respect to $1/Z$. Utilizing the CI method the relativistic Hamiltonian is specified within the no-pair approximation [13–15]. The corresponding contribution to the $M1$-transition probability is denoted by $\Delta W^{i\to f}_{\rm CI}$. The evaluation of this term is described in Sec. III.

The no-pair Hamiltonian does not account for the negative-energy excitations in the many-electron wave function. However, this effect, being dependent on the choice of the one-electron basis, can become significant [16,17]. In Sec. IV, the contribution due to the negative spectrum $\Delta W^{i\to f}_{\rm neg}$ is derived.

In Sec. V, the interelectronic-interaction correction of first order in $1/Z$ is evaluated within a rigorous QED approach employing the two-time Green function method [18]. Together with verifying the terms $\Delta W^{i\to f}_{\rm CI}$ and $\Delta W^{i\to f}_{\rm neg}$ to first order in $1/Z$, this provides the contribution $\Delta W^{i\to f}_{\rm freq}$, which incorporates the $1/Z$ interelectronic-interaction corrections of higher orders in αZ.

Finally, $\Delta W^{i\to f}_{\rm QED}$ is the QED correction. The evaluation of this correction to the lowest orders in α and αZ is described in Sec. VI.

The main goal of the present work is to evaluate the lifetimes of the states $(2s^22p)\ ^2P_{3/2}$ in B-like ions and $(2s2p)\ ^3P_2$ in Be-like ions to utmost accuracy and to investigate the influence of various effects on the $M1$-transition probability. The corresponding analysis is presented in Sec. VII.

Atomic units ($\hbar=e=m=1$) are used throughout the paper.

II. MAGNETIC-DIPOLE TRANSITION PROBABILITY

The spontaneous L-pole transition probability from the initial state i to the final state f reads [19]

$$W_L^{i\to f}=\frac{2\pi}{2J_i+1}\sum_{M_i}\sum_{M_f}\sum_{M}|A_{LM}|^2, \tag{1}$$

where the initial state has the angular momentum J_i, its z projection M_i, and the energy E_i, and J_f, M_f, and E_f denote the corresponding quantum numbers and the energy of the final state. The transition amplitude A_{LM} is defined as

$$A_{LM}=i^{L+1}\sqrt{\frac{\omega}{\pi c}}\sqrt{2L+1}\langle f|T_M^L|i\rangle. \tag{2}$$

Here T_M^L denote the components of the multipole transition operator $\mathbf{T}^L$, which is a spherical tensor of rank L. In the case of a magnetic transition, $\mathbf{T}^L$ is proportional to the tensor product of the Dirac-matrix vector $\boldsymbol{\alpha}$ and the spherical tensor $C_M^L=\sqrt{4\pi/(2L+1)}Y_{LM}$ [19],

$$T_M^L=-ij_L(\omega r/c)(\boldsymbol{\alpha}\otimes\mathbf{C}^L)_M^L, \tag{3}$$

where j_L is the spherical Bessel function and $\omega=E_i-E_f$ is the frequency of the emitted photon.

The magnetic transition probability can be expressed in terms of the reduced matrix element of T_M^L:

$$W_L^{i\to f}=\frac{2(2L+1)}{2J_i+1}\frac{\omega}{c}|\langle f\|\mathbf{T}^L\|i\rangle|^2. \tag{4}$$

For the magnetic-dipole transition ($L=1$), the tensor product can be written in terms of the vector product

$$\mathbf{T}^1=\frac{1}{\sqrt{2}}j_1(\omega r/c)\frac{[\boldsymbol{\alpha}\times\mathbf{r}]}{r}=\frac{\sqrt{2}}{r}j_1(\omega r/c)\boldsymbol{\mu}, \tag{5}$$

where $\boldsymbol{\mu}=-e[\mathbf{r}\times\boldsymbol{\alpha}]/2$ is the relativistic magnetic moment operator. Taking into account the first term in the expansion of $j_1(\omega r/c)$ only and turning into the nonrelativistic limit, one derives the following relation between the $M1$-transition operator $\mathbf{T}_{\rm nr}^1$ and the magnetic moment operator $\boldsymbol{\mu}_{\rm nr}$:

$$\mathbf{T}_{\rm nr}^1=\frac{\sqrt{2}}{3}\frac{\omega}{c}\boldsymbol{\mu}_{\rm nr}. \tag{6}$$

The nonrelativistic magnetic moment operator is given by

$$\boldsymbol{\mu}_{\rm nr}=-\mu_{\rm B}(\mathbf{L}+2\mathbf{S}), \tag{7}$$

where $\mathbf{L}$ and $\mathbf{S}$ are the orbital and spin angular momentum operators, respectively, and $\mu_{\rm B}=|e|\hbar/2mc$ denotes the Bohr magneton.

In the LS-coupling scheme, which is realized in the nonrelativistic case, the magnetic-dipole transition probability is nonzero only between fine-structure levels with $\Delta J=\pm1$ [12]. The reduced matrix element of $\mathbf{T}_{\rm nr}^1$ within the LS coupling is given by

$$\begin{aligned}\langle J_f\|\mathbf{T}_{\rm nr}^1\|J_i\rangle&=-\frac{\sqrt{2}}{3}\frac{\omega}{c}\mu_{\rm B}\langle J_f\|(\mathbf{J}+\mathbf{S})\|J_i\rangle\\&=-\frac{\sqrt{2}}{3}\frac{\omega}{c}\mu_{\rm B}\langle J_f\|\mathbf{S}\|J_i\rangle.\end{aligned} \tag{8}$$

Utilizing the general formula for the reduced matrix element of the spin operator [20] yields the corresponding expression for the transition probability:

$$\begin{aligned}W_{\rm nr}^{i\to f}=&\frac{4\omega^3}{3c^3}\mu_{\rm B}^2\delta_{L_i,L_f}\delta_{S_i,S_f}S_i(S_i+1)(2S_i+1)(2J_f+1)\\&\times\begin{Bmatrix}S_i & L_i & J_i\\ J_f & 1 & S_i\end{Bmatrix}^2.\end{aligned} \tag{9}$$

In particular, for the $2s^22p_{3/2}\to2s^22p_{1/2}$ transition one can easily find

$$W_{\rm nr}^{i\to f}=\frac{4\omega^3}{9c^3}\mu_{\rm B}^2=\frac{1}{3\lambda^3}2.6973500\times10^{13}\ {\rm s}^{-1}, \tag{10}$$

where λ is the transition wavelength in Å. Thus, in the nonrelativistic limit the magnetic-dipole transition probability is completely determined by the quantum numbers of the initial and final states.

III. INTERELECTRONIC INTERACTION IN THE BREIT APPROXIMATION

To evaluate the interelectronic-interaction contributions, we start with the relativistic Hamiltonian in the no-pair approximation,

$$H^{\rm np}=\Lambda_+H\Lambda_+,\quad H=\sum_i h^{\rm D}(i)+\sum_{i<j}V(i,j), \tag{11}$$

where $h^{\rm D}(i)$ is the one-particle Dirac Hamiltonian and the index $i=1,\ldots,N$ enumerates the electrons. The Coulomb-Breit interaction operator $V(i,j)=V_{\rm C}(i,j)+V_{\rm B}(i,j)$ is specified in coordinate space as

$$V_{\rm C}(i,j)=\frac{1}{r_{ij}},\quad V_{\rm B}(i,j)=-\frac{\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j}{r_{ij}}-\frac{1}{2}(\boldsymbol{\alpha}_i\cdot\boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_j\cdot\boldsymbol{\nabla}_j)r_{ij}. \tag{12}$$

The frequency-dependent part of the full QED interaction operator, which is beyond the Breit approximation and gives rise to the terms of higher orders in αZ, will be considered in Sec. V. Λ_+ is the projector on the positive-energy states, which can be represented as the product of the one-electron projectors $\lambda_+(i)$ as

$$\Lambda_+=\lambda_+(1)\cdots\lambda_+(N) \tag{13}$$

together with

$$\lambda_+(i)=\sum_n|u_n(i)\rangle\langle u_n(i)|. \tag{14}$$

Here u_n are the positive-energy eigenstates of an effective one-particle Hamiltonian h^u,

$$h^u u_n = \varepsilon_n u_n, \tag{15}$$

which can be taken to be the Dirac Hamiltonian h^{D}, the Dirac Hamiltonian in an external field or the Hartree-Fock-Dirac Hamiltonian in an external field [13–15].

In order to determine the space of one-electron functions $\{\varphi_n\}_{n=1}^{M}$, we employed the combined Dirac-Fock (DF) and the Dirac-Fock-Sturm (DFS) basis set. Here the index n enumerates different occupied and vacant one-electron states. For the occupied atomic shells, the orbitals φ_n with $n=1,\ldots,M_0$ were obtained by the standard restricted Dirac-Fock (RDF) method, based on a numerical solution of the radial RDF equations [21,22]. Only the Coulomb part $V_{\mathrm{C}}(i,j)$ of the Coulomb-Breit interaction operator (12) was included in the RDF Hamiltonian h^{DF}.

The vacant orbitals φ_n with $n=M_0+1,\ldots,M$ were obtained by solving the Dirac-Fock-Sturm equation

$$[h^{\mathrm{DF}} - \varepsilon_{n_0}]\varphi_n = \xi_n W(r)\varphi_n, \tag{16}$$

which can be considered as a generalization of the method proposed in Ref. [23] to the relativistic Hamiltonian and to an arbitrary constant-sign weight function $W(r)$. For every relativistic quantum number κ we choose an occupied DF function φ_{n_0}, which we call the reference DF orbital and ε_{n_0} in Eq. (16) is the energy of this orbital. The parameter ξ_n in Eq. (16) can be considered as an eigenvalue of the Sturmian operator. Obviously, for $\xi_n=0$ the Sturmian function coincides with the reference DF orbital φ_{n_0}. If $W(r)\to 0$ at $r\to\infty$, all Sturmian functions φ_n have the same exponential asymptotics at $r\to\infty$. Therefore, the whole set of eigenfunctions of the Dirac-Fock-Sturm operator forms a discrete set in the space of one-electron wave functions. The completeness of this basis in the nonrelativistic limit is a well-known fact. In the relativistic case this problem is more complicated and we examined the completeness of the pure DFS basis, which we used in our many-electron atomic calculations, numerically, reproducing exact hydrogenlike wave functions for the same nuclear charge number Z. It should be noted that the DFS orbitals are orthogonal with respect to the weight function $W(r)$ and, therefore, form a linear-independent basis set. The completeness and linear independence of the combined DF and DFS basis was also examined numerically.

In the nonrelativistic theory the widely used choice of the weight function is $W(r)=1/r$, which leads to the well-known "charge quantization." In the relativistic case, however, this choice is not very suitable, since the behavior of the Sturmian wave functions at the origin differs from that of the Dirac-Fock orbitals. In our calculations we employed the weight function

$$W(r) = \frac{1-\exp[-(\alpha r)^2]}{(\alpha r)^2}, \tag{17}$$

which, unlike $1/r$, is regular at the origin.

To generate the one-electron wave functions u_n, we used the unrestricted DF (UDF) method in the joined DF and DFS basis,

$$u_n = \sum_m C_{mn}\varphi_m. \tag{18}$$

The coefficients C_{mn} were obtained by solving the HFD matrix equations

$$\hat{F}\mathbf{C}_n = \varepsilon_n \hat{S}\mathbf{C}_n, \tag{19}$$

where $\hat{F}$ is the Dirac-Fock matrix in the joined basis of DF and DFS orbitals of a free ion. If necessary, an arbitrary external field can be included in the $\hat{F}$ matrix. The matrix $\hat{S}$ is nonorthogonal, since the DFS orbitals are not orthogonal in the usual sense. The negative-energy DFS functions were included in the total basis set as well. Equation (19) was used to generate the whole set of orthogonal one-electron wave functions $\{u_n\}_{n=1}^{M}$.

It should be noted that if even there is no external field in Eq. (19), the set of one-electron functions $\{u_n\}_{n=1}^{M}$ differs from the set of basis functions $\{\varphi_n\}_{n=1}^{M}$. For the occupied states, the UDF method accounts for core-polarization effects, in contrast to the RDF method. For the vacant states the difference is more significant, since the DF and DFS operators are inherently different.

The many-electron wave function $\Psi_+(\gamma J M_J)$ with quantum numbers γ, J, and M_J is expanded in terms of a large set of configuration state functions (CSF's) $\Phi_\alpha(JM_J)$:

$$\Psi_+(\gamma J M_J) = \Lambda_+\Psi(\gamma J M_J) = \sum_\alpha c_\alpha \Phi_\alpha(JM_J). \tag{20}$$

The standard configuration-interaction Dirac-Fock (CIDF) method is used to find the coefficients c_α. The CSF's are constructed from the one-electron wave functions u_n, Eq. (18), as a linear combination of Slater determinants. The set of the CSF's is generated including all single, double, and triple excitations into one-electron states of the positive spectrum.

IV. NEGATIVE-CONTINUUM CONTRIBUTION

Due to some freedom in the choice of wave function set $\{u_n\}$, the positive-energy subspace and the corresponding projector λ_+, Eq. (14), can be determined in different ways. This freedom can be used to find the optimum many-electron wave function Ψ_{opt} within the variational method.

The energy determined by Hamiltonian (11) can be written as

$$E = \langle\Psi|H^{\mathrm{np}}|\Psi\rangle = \langle\Psi_+|H|\Psi_+\rangle, \quad \Psi_+ = \Lambda_+\Psi. \tag{21}$$

The real orthogonal transformation (rotation) of the one-electron function space $\{u_n\}$ modifies the wave function Ψ_+ [24],

$$\Psi' = \exp(T)\Psi_+, \tag{22}$$

where the operator T is anti-Hermitian ($T^\dagger=-T$),

$$T = \sum_{n<m} E_{nm}t_{nm}, \quad E_{nm} = a_n^\dagger a_m - a_m^\dagger a_n. \tag{23}$$

Here $a_n^\dagger$ and a_n are the creation and annihilation operators of electron in the u_n state. The matrix elements t_{nm} can be ob-

tained from the variational principle. Then the wave function $\Psi_{\rm opt}$ satisfies the generalized Brillouin theorem [25]

$$\langle\Psi_{\rm opt}|[a_n^\dagger a_m, H]|\Psi_{\rm opt}\rangle = 0. \tag{24}$$

This means that the optimum wave function $\Psi_{\rm opt}$ is invariable under single excitations including negative-energy spectrum excitations. However, this does not hold for the wave function Ψ_+. Therefore, one should revise the calculation of the matrix element $\langle\Psi_+|A|\Psi_+\rangle$ of any one-electron operator A by admixing the negative-energy spectrum excitations to Ψ_+. This is especially important for so-called "odd" operators, which mix the large and small components of the Dirac wave functions. The $M1$-transition operator $\mathbf{T}^1$, Eq. (5), is just of this kind. For this reason, the negative-continuum contribution can be significant and depends on the choice of the one-electron basis set $\{u_n\}$ [16,17].

We consider two equivalent methods for evaluating the negative-continuum contribution to the matrix elements of a hermitian one-electron operator A with the wave functions Ψ_+. The first one is based on the Hellman-Feynman theorem whereas the second one employs the perturbation theory.

The space of the wave functions used to find $\Psi_{\rm opt}$ is invariant under the transformation $U=\exp(iA)$, if A is a one-particle operator. Therefore, one can employ the Hellman-Feynman theorem [26] to obtain the expectation value of A,

$$\overline{A} = \left.\frac{\partial}{\partial\mu}\langle\Psi_{\rm opt}(\mu)|H(\mu)|\Psi_{\rm opt}(\mu)\rangle\right|_{\mu=0}, \quad H(\mu) = H + \mu A, \tag{25}$$

where it is implied that μA is included in the one-particle Hamiltonian, $h^u(\mu)=h^u+\mu A$. Since the wave function correction

$$\delta\Psi = \Psi_{\rm opt} - \Psi_+ = [1-\exp(-T)]\Psi_{\rm opt} \simeq -\sum_{n<m} E_{nm}t_{nm}\Psi_{\rm opt} \tag{26}$$

accounts for single excitations only, the generalized Brillouin theorem (24) yields

$$\langle\delta\Psi(\mu)|H(\mu)|\Psi_{\rm opt}(\mu)\rangle + \langle\Psi_{\rm opt}(\mu)|H(\mu)|\delta\Psi(\mu)\rangle = 0 \tag{27}$$

and, therefore,

$$\overline{A} = \frac{\partial}{\partial\mu}[\langle\Psi_+(\mu)|H(\mu)|\Psi_+(\mu)\rangle - \langle\delta\Psi(\mu)|H(\mu)|\delta\Psi(\mu)\rangle]_{\mu=0}. \tag{28}$$

Neglecting the second quadratic term in the equation above yields

$$\overline{A} \simeq \frac{\partial}{\partial\mu}[\langle\Psi_+(\mu)|H(\mu)|\Psi_+(\mu)\rangle]_{\mu=0}. \tag{29}$$

Thus, the negative-continuum contribution can be evaluated by means of the formula

$$\Delta\overline{A}_{\rm neg} = \frac{\partial}{\partial\mu}[\langle\Psi_+(\mu)|H(\mu)|\Psi_+(\mu)\rangle]_{\mu=0} - \langle\Psi_+|A|\Psi_+\rangle. \tag{30}$$

An alternative expression for this contribution can be obtained employing the perturbation theory. Using the equation for the derivative of $u_n(\mu)$,

$$\left.\frac{\partial}{\partial\mu}u_n(\mu)\right|_{\mu=0} = \sum_{m\neq n}\frac{\langle u_m(0)|A|u_n(0)\rangle}{\varepsilon_n-\varepsilon_m}u_m(0), \tag{31}$$

we obtain

$$\Delta\overline{A}_{\rm neg} = 2\sum_n^{\rm (pos)}\sum_m^{\rm (neg)}\frac{\langle u_m|A|u_n\rangle}{\varepsilon_n-\varepsilon_m}\langle a_m^\dagger a_n\Psi_+|H|\Psi_+\rangle. \tag{32}$$

Here the indices (pos) and (neg) indicate that the summation is carried out over the positive- and negative-energy spectra, respectively.

For the nondiagonal matrix elements, one can derive

$$\Delta A_{\rm neg}^{i\to f} = \frac{\partial}{\partial\mu}[\langle\Psi_+^f(\mu)|H(\mu)|\Psi_+^i(\mu)\rangle]_{\mu=0} - \langle\Psi_+^f|A|\Psi_+^i\rangle \tag{33}$$

and

$$\Delta A_{\rm neg}^{i\to f} = \sum_n^{\rm (pos)}\sum_m^{\rm (neg)}\frac{\langle u_m|A|u_n\rangle}{\varepsilon_n-\varepsilon_m} \times [\langle a_m^\dagger a_n\Psi_+^f|H|\Psi_+^i\rangle + \langle\Psi_+^f|H|a_m^\dagger a_n\Psi_+^i\rangle]. \tag{34}$$

These formulas were used in our calculations of the negative-continuum contribution to the $M1$-transition amplitude. It was found that the results obtained by means of Eqs. (33) and (34) are in a perfect agreement with each other.

V. HIGHER-ORDER INTERELECTRONIC-INTERACTION CORRECTIONS

A rigorous QED treatment of the interelectronic-interaction corrections to the transition probabilities can be carried out utilizing the two-time Green function method [18]. In Ref. [27] it was done for the $1/Z$ interelectronic-interaction corrections in He-like ions. Here we perform the corresponding calculations for B-like ions. To simplify the derivation of formal expressions, we specify the formalism regarding the core electrons as belonging to a redefined vacuum (for details we refer to Refs. [18,28]). This leads to merging the interelectronic-interaction corrections of order $1/Z$ with the one-loop radiative corrections. The formulas for these corrections can easily be obtained from the corresponding expressions for the one-loop radiative corrections to the transition amplitude in a one-electron atom, derived in [18]. However, the standard electron propagator $S(\varepsilon,\mathbf{x},\mathbf{y})$, which enters the equations, must be replaced by

$$\widetilde{S}(\varepsilon,\mathbf{x},\mathbf{y}) = S(\varepsilon,\mathbf{x},\mathbf{y}) + 2\pi i \sum_c \psi_c(\mathbf{x})\bar{\psi}_c(\mathbf{y})\delta(\varepsilon-\varepsilon_c), \quad (35)$$

where the summation runs over all occupied one-electron states referring to the closed shells. Accordingly, the total expression is represented by the sum of the pure QED and interelectronic-interaction contributions, which correspond to the first and second terms on the right-hand side of Eq. (35). As a result, the $1/Z$ interelectronic-interaction correction to the $M1$-transition amplitude in a B-like ion between the initial state a and the final state b is

$$\begin{aligned}\Delta A_{1M}^{\mathrm{int}} = &-\sqrt{\frac{\omega}{\pi c}}\sqrt{3}\sum_c \Bigg\{ \sum_{n\neq b} \frac{\langle bc|I(0)|nc\rangle\langle n|T_M^1|a\rangle}{\varepsilon_b-\varepsilon_n} \\ &+ \sum_{n\neq a} \frac{\langle b|T_M^1|n\rangle\langle cn|I(0)|ca\rangle}{\varepsilon_a-\varepsilon_n} \\ &+ \sum_n \frac{\langle bc|I(\varepsilon_a-\varepsilon_b)|an\rangle\langle n|T_M^1|c\rangle}{\varepsilon_b+\varepsilon_c-\varepsilon_a-\varepsilon_n} \\ &+ \sum_n \frac{\langle c|T_M^1|n\rangle\langle nb|I(\varepsilon_a-\varepsilon_b)|ca\rangle}{\varepsilon_a+\varepsilon_c-\varepsilon_b-\varepsilon_n} \\ &- \sum_{n\neq b} \frac{\langle bc|I(\varepsilon_b-\varepsilon_c)|cn\rangle\langle n|T_M^1|a\rangle}{\varepsilon_b-\varepsilon_n} \\ &- \sum_{n\neq a} \frac{\langle b|T_M^1|n\rangle\langle nc|I(\varepsilon_a-\varepsilon_c)|ca\rangle}{\varepsilon_a-\varepsilon_n} \\ &- \sum_n \frac{\langle bc|I(\varepsilon_a-\varepsilon_c)|na\rangle\langle n|T_M^1|c\rangle}{\varepsilon_b+\varepsilon_c-\varepsilon_a-\varepsilon_n} \\ &- \sum_n \frac{\langle c|T_M^1|n\rangle\langle bn|I(\varepsilon_b-\varepsilon_c)|ca\rangle}{\varepsilon_a+\varepsilon_c-\varepsilon_b-\varepsilon_n} - \frac{1}{2}\langle b|T_M^1|a\rangle \\ &\times[\langle bc|I'(\varepsilon_b-\varepsilon_c)|cb\rangle + \langle ac|I'(\varepsilon_a-\varepsilon_c)|ca\rangle]\Bigg\}, \end{aligned} \quad (36)$$

where $I(\varepsilon)=\alpha^\mu\alpha^\nu D_{\mu\nu}(\varepsilon)$, $I'(\varepsilon)=\mathrm{d}I(\varepsilon)/\mathrm{d}\varepsilon$, $\alpha^\mu=(1,\boldsymbol{\alpha})$, and $D_{\mu\nu}(\varepsilon)$ is the photon propagator. In the Feynman gauge it reads

$$D_{\mu\nu}(\varepsilon,\mathbf{x}-\mathbf{y}) = -4\pi g_{\mu\nu}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\exp[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})]}{\varepsilon^2-\mathbf{k}^2+i0}, \quad (37)$$

where $g_{\mu\nu}$ is the metric tensor. In the Coulomb gauge we have

$$D_{00}(\varepsilon,\mathbf{x}-\mathbf{y}) = \frac{1}{|\mathbf{x}-\mathbf{y}|}, \quad D_{i0}=D_{0i}=0, \quad (i=1,2,3),$$

$$D_{ij}(\varepsilon,\mathbf{x}-\mathbf{y}) = 4\pi\int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\exp[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})]}{\varepsilon^2-\mathbf{k}^2+i0}\left(\delta_{i,j}-\frac{k_ik_j}{\mathbf{k}^2}\right), \quad (i,j=1,2,3). \quad (38)$$

In contrast to Ref. [18], here atomic units and the Gauss charge unit ($\alpha=e^2/\hbar c$) are used. Expression (36) incorporates the Coulomb-Breit part, which was taken into account by the CI method, together with terms of higher order in αZ, the so-called frequency-dependent correction. Specifying the operator $I(\varepsilon)$ within the Coulomb gauge and setting $\varepsilon=0$ in Eq. (36) yields the Coulomb-Breit interaction. In this way we can exclude the part which has already been taken into account by the CI method and obtain the frequency-dependent correction of order $1/Z$ as

$$\begin{aligned}\Delta A_{1M}^{\mathrm{freq}} = &\sqrt{\frac{\omega}{\pi c}}\sqrt{3}\sum_c \Bigg\{ \sum_{n\neq b} \frac{\langle bc|\Delta I_{\mathrm{C}}(\varepsilon_b-\varepsilon_c)|cn\rangle\langle n|T_M^1|a\rangle}{\varepsilon_b-\varepsilon_n} \\ &+ \sum_{n\neq a} \frac{\langle b|T_M^1|n\rangle\langle nc|\Delta I_{\mathrm{C}}(\varepsilon_a-\varepsilon_c)|ca\rangle}{\varepsilon_a-\varepsilon_n} \\ &+ \sum_n \frac{\langle bc|\Delta I_{\mathrm{C}}(\varepsilon_a-\varepsilon_c)|na\rangle\langle n|T_M^1|c\rangle}{\varepsilon_b+\varepsilon_c-\varepsilon_a-\varepsilon_n} \\ &+ \sum_n \frac{\langle c|T_M^1|n\rangle\langle bn|\Delta I_{\mathrm{C}}(\varepsilon_b-\varepsilon_c)|ca\rangle}{\varepsilon_a+\varepsilon_c-\varepsilon_b-\varepsilon_n} \\ &- \sum_n \frac{\langle bc|\Delta I_{\mathrm{C}}(\varepsilon_a-\varepsilon_b)|an\rangle\langle n|T_M^1|c\rangle}{\varepsilon_b+\varepsilon_c-\varepsilon_a-\varepsilon_n} \\ &- \sum_n \frac{\langle c|T_M^1|n\rangle\langle nb|\Delta I_{\mathrm{C}}(\varepsilon_a-\varepsilon_b)|ca\rangle}{\varepsilon_a+\varepsilon_c-\varepsilon_b-\varepsilon_n} + \frac{1}{2}\langle b|T_M^1|a\rangle \\ &\times[\langle bc|I'_{\mathrm{C}}(\varepsilon_b-\varepsilon_c)|cb\rangle + \langle ac|I'_{\mathrm{C}}(\varepsilon_a-\varepsilon_c)|ca\rangle]\Bigg\}, \end{aligned} \quad (39)$$

where $\Delta I_{\mathrm{C}}(\varepsilon_a-\varepsilon_b)=I_{\mathrm{C}}(\varepsilon_a-\varepsilon_b)-I_{\mathrm{C}}(0)$ and the subscript "C" refers to the Coulomb gauge.

It should be noted that the total $1/Z$ interelectronic-interaction correction given by Eq. (36) is gauge independent. This has been confirmed in our calculations to a very high accuracy. The calculations were performed employing the B-spline method for the Dirac equation [29].

VI. QED CORRECTION

QED effects modify the transition probability via the matrix element of the transition operator and via the transition energy. Since we employ the experimental value for the transition energy, we have to consider the QED effect on the transition amplitude only.

The lowest-order QED correction to the $M1$-transition amplitude can be derived by correcting the operator of the atomic magnetic moment for the anomalous magnetic moment of a free electron. In the nonrelativistic limit it yields

$$\boldsymbol{\mu}_{\mathrm{nr}} \to \boldsymbol{\mu}_a = -\mu_{\mathrm{B}}[\mathbf{L}+2(1+\kappa_e)\mathbf{S}] = \boldsymbol{\mu}_{\mathrm{nr}} + \delta\boldsymbol{\mu}_a, \quad (40)$$

where

$$\delta\boldsymbol{\mu}_a = -2\mu_{\mathrm{B}}\kappa_e\mathbf{S}, \quad (41)$$

$$\kappa_e = \left[\frac{\alpha}{2\pi} - 0.328\,478\,965\ldots\left(\frac{\alpha}{\pi}\right)^2 + \cdots\right]. \quad (42)$$

With the aid of the identity

TABLE I. The decay rates W (s^{-1}) of the magnetic-dipole transition $(1s^22s^22p)\ ^2P_{1/2}-^2P_{3/2}$ and the lifetimes τ (ms) of the $(1s^22s^22p)\ ^2P_{3/2}$ state in B-like ions. Numbers in the parentheses give the estimated error.

	S^{11+}	Cl^{12+}	Ar^{13+}	K^{14+}	Ti^{17+}
Energy (cm^{-1})	13135(1)	17408(20)	22656.22(1)	29006(25)	56243(4)
W_{nr}	20.37538	47.43068	104.56308	219.4222	1599.635
ΔW_D	−0.03542	−0.09302	−0.23145	−0.5436	−5.355
ΔW_{CI}	0.00637	0.01586	0.03723	0.0802	0.597
ΔW_{neg}	−0.00159	−0.00396	−0.00929	−0.0206	−0.176
ΔW_{QED}	0.09451	0.22001	0.48502	1.0178	7.420
ΔW_{freq}	0.00007	0.00019	0.00049	0.0012	0.013
W_{total}	20.439(5)	47.57(16)	104.85(2)	220.0(6)	1602.1(5)
τ_{total}	48.93(1)	21.02(7)	9.538(2)	4.546(12)	0.6242(2)

$$\langle J_f \| \mathbf{J} \| J_i \rangle = \langle J_f \| (\mathbf{L}+\mathbf{S}) \| J_i \rangle = \delta_{J_f,J_i} \sqrt{J_i(J_i+1)(2J_i+1)}, \tag{43}$$

one can easily find for the fine-structure level transition ($\Delta J = \pm 1$)

$$\langle J_f \| \delta \boldsymbol{\mu}_a \| J_i \rangle = 2\kappa_e \langle J_f \| \boldsymbol{\mu}_{nr} \| J_i \rangle. \tag{44}$$

Therefore, the QED correction to the $M1$-transition probability is given by

$$\Delta W^{i\to f}_{QED} = \frac{4\omega^3}{3c^3}\frac{1}{2J_i+1}\left[\left|\langle J_f \| (\boldsymbol{\mu}_{nr}+\delta\boldsymbol{\mu}_a) \| J_i \rangle\right|^2 - \left|\langle J_f \| \boldsymbol{\mu}_{nr} \| J_i \rangle\right|^2\right], \tag{45}$$

which yields

$$\Delta W^{i\to f}_{QED} \simeq 4\kappa_e \frac{4\omega^3}{3c^3}\frac{1}{2J_i+1}\left|\langle J_f \| \boldsymbol{\mu}_{nr} \| J_i \rangle\right|^2 \simeq 4\kappa_e W^{i\to f}_{nr}. \tag{46}$$

QED corrections, which are not accounted for by this formula, are suppressed by a small factor $(\alpha Z)^2$.

VII. RESULTS AND DISCUSSION

The individual contributions to the $M1$-transition probabilities and the corresponding lifetimes for B-like and Be-like ions are presented in Tables I and II, respectively. Due to the smallness of the $E2$ transition, which is also allowed, the lifetimes are essentially determined by the $M1$ transition. In case of B-like ions, the experimental values of the transition energy were taken from Ref. [30] for S^{11+}, Cl^{12+}, K^{14+}, and Ti^{17+} and from Ref. [31] for Ar^{13+}. As one can see from Table I the interelectronic-interaction correction ΔW_{CI} turns out to be relatively small due to the smallness of the factor $(\alpha Z)^2/Z$. The most important contributions are given by the relativistic correction ΔW_D and by the QED correction ΔW_{QED}. For Be-like ions, the transition energies were taken from Ref. [32] for S^{12+}, Cl^{13+}, K^{15+}, and Ti^{18+} and from Ref. [31] for Ar^{14+}. In this case the interelectronic-interaction correction ΔW_{CI} provides an essential contribution to the total value of the transition probability. This is due to a strong mixing of the two terms $^3P_1$ and $^1P_1$. Except for Ar^{13+} and Ar^{14+}, the uncertainties of the total transition probabilities are mainly determined by the experimental uncertainties of the transition energy. For argon ions, the uncertainty comes mainly from uncalculated higher-order QED corrections.

In Table III, our results for the lifetime of the $(1s^22s^22p)\ ^2P_{3/2}$ state are compared with other calculations and with

TABLE II. The decay rates W (s^{-1}) of the magnetic-dipole transition $(1s^22s2p)\ ^3P_1-^3P_2$ and the lifetimes τ (ms) of the $(1s^22s2p)\ ^3P_2$ state in Be-like ions. Numbers in the parentheses give the estimated error.

	S^{12+}	Cl^{13+}	Ar^{14+}	K^{15+}	Ti^{18+}
Energy (cm^{-1})	9712(14)	12913(16)	16819.36(1)	21571(20)	42638(4)
W_{nr}	12.35488	29.03947	64.17056	135.36899	1045.4311
ΔW_D	−0.02017	−0.05389	−0.13242	−0.31247	−3.2611
ΔW_{CI}	−0.01302	−0.04909	−0.16457	−0.50484	−10.0481
ΔW_{neg}	−0.00053	−0.00133	−0.00313	−0.00704	−0.0649
ΔW_{QED}	0.05731	0.13470	0.29766	0.62792	4.8493
W_{total}	12.38(5)	29.07(11)	64.17(1)	135.2(4)	1036.9(4)
τ_{total}	80.79(33)	34.40(13)	15.584(2)	7.398(22)	0.9645(4)

TABLE III. The lifetimes of the $(1s^22s^22p)\ ^2P_{3/2}$ level in B-like ions calculated in this work with (τ_{pres}) and without (τ^0_{pres}) the QED correction are compared with previous calculations (τ_{theor}) and experiment (τ_{expt}). The lifetime values are given in ms. The values of the transition energy [Energy] are presented in cm^{-1}. Numbers in the parentheses give the estimated error. MCDF, multiconfiguration Dirac-Fock method; MCBP, multiconfiguration Breit-Pauli method; SS, SUPERSTRUCTURE program; MRCI, multireference relativistic configuration interaction method; RQDO, relativistic quantum defect orbital method.

Ions	τ^0_{pres}	τ_{pres} [Energy]	τ_{theor} [Energy]	Method and ref.	τ_{expt} and Ref.
S^{11+}	49.16	48.93(1) [13135]	47.35 [13300]	MCDF [9]	
			49.07 [13115]	MCBP [10]	
			49.33 [13144]	MCDF [33]	
			49.07 [13136]	SS [34]	
			49.26 [13122]	MRCI [35]	
			49.60	RQDO [11]	
Cl^{12+}	21.12	21.02(7) [17408]	20.55 [17565]	MCDF [9]	21.2(6) [6]
			21.02 [17400]	MCBP [10]	21.1(5) [6]
			21.19 [17421]	MCDF [33]	
			21.08 [17410]	SS [34]	
			21.19 [17386]	MRCI [35]	
			21.13	RQDO [11]	
Ar^{13+}	9.582	9.538(2) [22656]	9.407 [22795]	MCDF [9]	8.7(5) [38]
			9.515 [22660]	MCBP [10]	9.12(18) [2]
			9.618 [22666]	MCDF [33]	9.70(15) [4]
			9.569 [22653]	SS [34]	9.573(4)(5) [8]
			9.588 [22657]	RQDO [11]	
			9.606 [22636]	MCDF [36]	
			9.615 [22619]	MRCI [35]	
			9.534 [22658]	[37]	
K^{14+}	4.567	4.546(12) [29006]	4.509 [29129]	MCDF [9]	4.47(10) [5]
			4.521 [29044]	MCBP [10]	
			4.583 [29019]	MCDF [33]	
			4.558 [29004]	SS [34]	
			4.587 [28960]	MRCI [35]	
			4.577	RQDO [11]	
Ti^{17+}	0.6271	0.6242(2) [56243]	0.6254 [56275]	MCDF [9]	0.627(10) [3]
			0.6150 [56465]	MCBP [10]	
			0.6290 [56258]	MCDF [33]	
			0.6254 [56240]	SS [34]	
			0.6289 [56166]	MRCI [35]	
			0.6270	RQDO [11]	

experiment. It should be noted that the QED correction was taken into account in Refs. [10,37] and in the present work only. Besides, different values of the transition energy ω, indicated in Table III, were used in the different calculations. Since the $M1$-transition probability W scales as ω^3, a small deviation in ω can change W significantly. For this reason, we recalculated the results of Cheng *et al.* [9] and Fischer [10] for the $(1s^22s^22p)\ ^2P_{3/2}$ state in B-like ions for those transition energies we have employed in our calculations. Table IV presents these values with (τ [10]) and without (τ^0 [9]) the anomalous magnetic moment correction and the corresponding values (τ_{pres} and τ^0_{pres}) obtained in this work. As one can see from the table, there is excellent agreement be-

TABLE IV. The lifetimes of the $(1s^22s^22p)\ ^2P_{3/2}$ level in B-like ions calculated in this work with (τ_{pres}) and without (τ^0_{pres}) the QED correction are compared with previous theoretical results, recalculated to the transition energy [Energy (cm^{-1})] employed in this paper. The lifetime values are given in ms.

Ions	Energy	τ^0_{pres}	τ^0 [9]	τ_{pres}	τ [10]
S^{11+}	13135	49.16	49.16	48.93	48.85
Cl^{12+}	17408	21.12	21.11	21.02	20.99
Ar^{13+}	22656	9.582	9.581	9.538	9.520
K^{14+}	29006	4.567	4.567	4.546	4.539
Ti^{17+}	56243	0.6271	0.6265	0.6242	0.6223

TABLE V. The lifetimes of the $(1s^22s2p)\ ^3P_2$ level in Be-like ions calculated in this work with (τ_{pres}) and without (τ^0_{pres}) the QED correction are compared with previous calculations (τ_{theor}) and experiment (τ_{expt}). The lifetime values are given in ms. The values of the transition energy [Energy] are presented in cm^{-1}. Numbers in the parentheses give the estimated error. SHF, scaled Hartree-Fock method; MBPT, many-body perturbation theory; MCHF, multiconfiguration Hartree-Fock method; MCDF, multiconfiguration Dirac-Fock method.

Ions	τ^0_{pres}	τ_{pres} [Energy]	τ_{theor} [Energy]	Method and Ref.	τ_{expt} and Ref.
S^{12+}	81.16	80.79(33) [9712]	83.3 [9743]	SHF [39]	
			80.65 [9720]	MBPT [40]	
Cl^{13+}	34.56	34.40(13) [12913]	35.7 [12893]	SHF [39]	
			34.60 [12903]	MBPT [40]	
Ar^{14+}	15.66	15.584(2) [16819]	16.31 [16818]	MCHF [41]	15.0(7) [1]
			16.1 [16824]	SHF [39]	13.4(7) [2]
			15.63 [16834]	MBPT [40]	15.0(8) [4]
			15.76 [16782]	MCDF [36]	
K^{15+}	7.432	7.398(22) [21571]	7.63 [21575]	SHF [39]	7.6(5) [5]
			7.353 [21633]	MBPT [40]	
Ti^{18+}	0.9689	0.9645(4) [42638]	0.990 [42653]	SHF [39]	
			0.9615 [42651]	MBPT [40]	

tween our "non-QED" results (τ^0_{pres}) and those from Ref. [9] (τ^0). There is also good agreement between our total results (τ_{pres}) and those from Ref. [10] (τ). The comparison of our theoretical results with the experimental data shows generally a good agreement as well. However, in case of Ar^{13+} there is a discrepancy between our $^2P_{3/2}$ lifetime value 9.538(2) ms and the most accurate experimental value 9.573(4)(5) ms [7,8].

Table V shows a fair agreement of our results for the lifetime of the $(1s^22s2p)\ ^3P_2$ state in Be-like ions with corresponding results obtained by other authors and with experimental data. We note that the QED correction has not been considered in the previous calculations cited in the table.

In conclusion, we have evaluated the magnetic-dipole transition probabilities between the fine-structure levels $(1s^22s^22p)\ ^2P_{1/2}-^2P_{3/2}$ for B-like ions and $(1s^22s2p)\ ^3P_1-^3P_2$ for Be-like ions. The relativistic, interelectronic-interaction, and radiative corrections to the transition probability have been considered. Except for a recent high-precision lifetime measurement on Ar^{13+} [7,8] with an accuracy level on the order of 0.1%, most experimental results have large error bars greater than 1.5% and, within these error bars, most of them are in fair agreement with our theoretical predictions. In case of Ar^{13+}, the disagreement of our prediction with the high-precision experimental value amounts to 0.37% of the total transition probability, less than the value of the corresponding QED correction. At present we have no explanation for this discrepancy.

ACKNOWLEDGMENTS

Valuable conversations with O. Yu. Andreev are gratefully acknowledged. This work was supported in part by RFBR (Grant No. 04-02-17574), INTAS-GSI (Grant No. 03-54-3604), and the Russian Ministry of Education. D.A.G. acknowledges financial support from the foundation "Dynasty." A.V.V. and G.P. acknowledge financial support from the GSI F+E program, DFG, and BMBF. The work of A.V.V. was also supported by DAAD and the "Dynasty" foundation.

[1] T. V. Back, H. S. Margolis, P. K. Oxley, J. D. Silver, and E. G. Myers, Hyperfine Interact. **114**, 203 (1998).
[2] D. P. Moehs and D. A. Church, Phys. Rev. A **58**, 1111 (1998).
[3] E. Träbert G. Gwinner, A. Wolf, X. Tordoir, and A. G. Calamai, Phys. Lett. A **264**, 311 (1999).
[4] E. Träbert, P. Beiersdorfer, S. B. Utter, G. V. Brown, H. Chen, C. L. Harris, P. A. Neill, D. W. Savin, and A. J. Smith, Astrophys. J. **541**, 506 (2000).
[5] E. Träbert, P. Beiersdorfer, G. V. Brown, H. Chen, E. H. Pinnington, and D. B. Thorn, Phys. Rev. A **64**, 034501 (2001).
[6] E. Träbert, P. Beiersdorfer, G. Gwinner, E. H. Pinnington, and A. Wolf, Phys. Rev. A **66**, 052507 (2002).
[7] J. R. Crespo López-Urrutia, A. N. Artemyev, J. Braun, G. Brenner, H. Bruhns, I. N. Draganić, A. J. González Martínez, A. Lapierre, V. Mironov, J. Scofield, R. Soria Orts, H. Tawara, M. Trinczek, I. I. Tupitsyn, and J. Ullrich, Nucl. Instrum. Methods Phys. Res. B **235**, 85 (2005).
[8] A. Lapierre, U. D. Jentschura, J. R. Crespo López-Urrutia, J. Braun, G. Brenner, H. Bruhns, D. Fischer, A. J. González Martínez, Z. Harman, W. R. Johnson, C. H. Keitel, V. Mironov, C. J. Osborne, G. Sikler, R. Soria Orts, V. M. Sha-

baev, H. Tawara, I. I. Tupitsyn, J. Ullrich, and A. Volotka, Phys. Rev. Lett. (to be published).
[9] K. T. Cheng, Y. -K. Kim, and J. P. Desclaux, At. Data Nucl. Data Tables **24**, 111 (1979).
[10] C. F. Fischer, J. Phys. B **16**, 157 (1983).
[11] E. Charro, S. López-Ferrero, and I. Martín, J. Phys. B **34**, 4243 (2001).
[12] I. I. Sobelman, *Atomic Spectra and Radiative Transitions* (Springer, New York, 1979).
[13] J. Sucher, Phys. Rev. A **22**, 348 (1980).
[14] M. H. Mittleman, Phys. Rev. A **24**, 1167 (1981).
[15] D. A. Glazov, V. M. Shabaev, I. I. Tupitsyn, A. V. Volotka, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. A **70**, 062104 (2004).
[16] P. Indelicato, Phys. Rev. Lett. **77**, 3323 (1996).
[17] A. Derevianko, I. M. Savukov, W. R. Johnson, and D. R. Plante, Phys. Rev. A **58**, 4453 (1998).
[18] V. M. Shabaev, Phys. Rep. **356**, 119 (2002).
[19] I. P. Grant, J. Phys. B **7**, 1458 (1974).
[20] D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii, *Quantum Theory of Angular Momentum* (World Scientific, Singapore, 1988).
[21] I. P. Grant, Adv. Phys. **19**, 747 (1970).
[22] V. F. Bratzev, G. B. Deyneka, and I. I. Tupitsyn, Bull. Acad. Sci. USSR, Phys. Ser. (Engl. Transl.) **41**, 2655 (1977) [Bull. Acad. Sci. USSR, Phys. Ser. (Engl. Transl.) **41**, 173 (1977)].
[23] P. F. Gruzdev, G. S. Soloveva, and A. I. Sherstyuk, Opt. Spectrosc. **42**, 1198 (1977) [Opt. Spectrosc. **42**, 690 (1977)].
[24] E. Dalgaard and P. Jørgensen, J. Chem. Phys. **69**, 3833 (1978).
[25] B. Levy and G. Berthier, Int. J. Quantum Chem. **2**, 307 (1968).
[26] S. T. Epstein, *Variation Method in Quantum Chemistry* (Academic Press, New York, 1974).
[27] P. Indelicato, V. M. Shabaev, and A. V. Volotka, Phys. Rev. A **69**, 062506 (2004).
[28] M. B. Shabaeva and V. M. Shabaev, Phys. Rev. A **52**, 2811 (1995).
[29] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 307 (1988).
[30] B. Edlén, Phys. Scr. **28**, 483 (1983).
[31] I. Draganić, J. R. Crespo López-Urrutia, R. DuBois, S. Fritzsche, V. M. Shabaev, R. Soria Orts, I. I. Tupitsyn, Y. Zou, and J. Ullrich, Phys. Rev. Lett. **91**, 183001 (2003).
[32] B. Edlén, Phys. Scr. **28**, 51 (1983).
[33] T. R. Verhey, B. P. Das, and W. F. Perger, J. Phys. B **20**, 3639 (1987).
[34] M. E. Galavís, C. Mendoza, and C. J. Zeippen, Astron. Astrophys., Suppl. Ser. **131**, 499 (1998).
[35] K. Koc, J. Phys. B **36**, L93 (2003).
[36] C. Z. Dong, S. Fritzsche, B. Fricke, and W. -D. Sepp, Phys. Scr. **T92**, 294 (2001).
[37] W. R. Johnson (private communication).
[38] F. G. Serpa, J. D. Gillaspy, and E. Träbert, J. Phys. B **31**, 3345 (1998).
[39] V. Kaufman and J. Sugar, J. Phys. Chem. Ref. Data **15**, 321 (1986).
[40] U. I. Safronova, W. R. Johnson, and A. Derevianko, Phys. Scr. **60**, 46 (1999).
[41] R. Glass, Astrophys. Space Sci. **91**, 417 (1983).